1D-CNN model development for soluble solids content evaluation of apple using Vis/NIR spectroscopy

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2. Materials and Methods

3. Results and Discussion

4. Conclusions



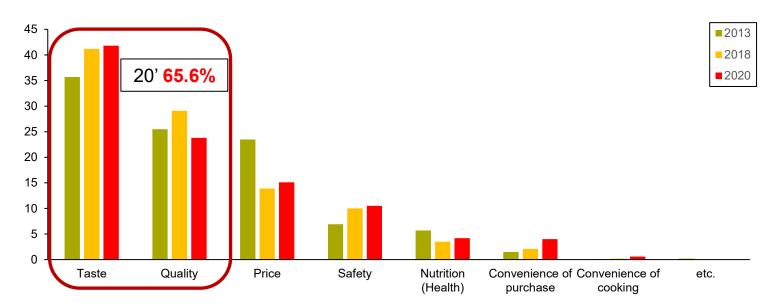




- Apple: The most cultivated fruit among Korea's representative fruits and the most favored by consumers
- Consumers demand high internal quality agricultural produce

Fruit sorting: very important as an essential process not only to improve value-added but also
to guarantee the quality of agricultural products, standardization, and improve distribution

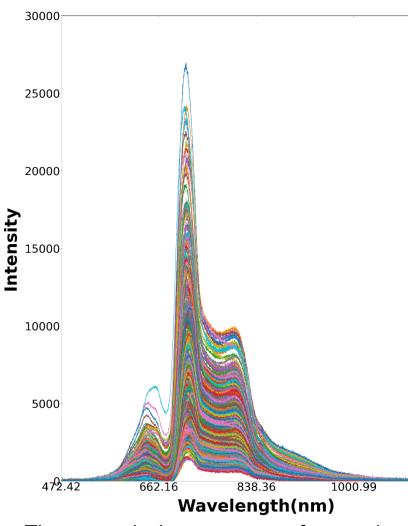
efficiency.



Quality factor

- External quality
 - : Size, color, weight, shape, external defect, etc.
- Internal quality
 - : Sugar, acidity, moisture content, internal defects, etc.
- Determination of Internal quality: Near-infrared spectroscopy
- Near-infrared(NIR) spectroscopy

: A technique for calculating the sugar content by **measuring** transmitted or reflected light with a spectrometer when NIR rays (700 to 2500 nm) are applied to a fruit.



The transmission spectrum of an apple

Spectroscopic mode

Reflectance mode

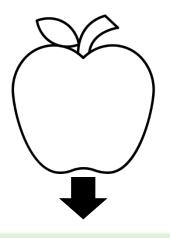
: Using reflected light on the fruit surface Simple structure, only the components of the surface can be measured

b. Full-transmittance mode

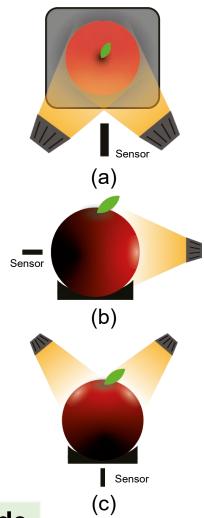
: Using light that penetrates the entire interior of the fruit Overall component of the fruit can be measured, but the amount of light transmitted is small

c. Semi-transmittance mode

: Use of light via part of the inside of the fruit Overall component of fruit can be measured, the amount of light transmitted is large, but a lot of light is required



Full/Semi-transmittance mode is commonly used in apple



Fruit : 90%(water), Others(sugar, acid, etc.)

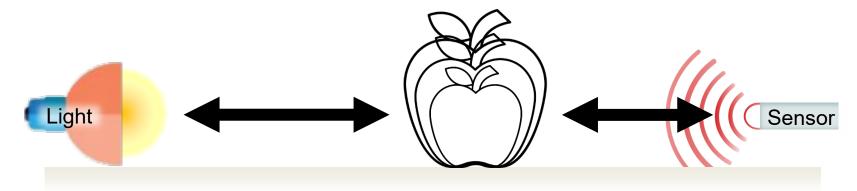


- → Sugar and acid components cannot cause significant variations in the transmission spectrum Changes in the optical path due to differences in sample size, etc. cause greater
- Currently, the spectroscopic measurement unit of the non-destructive sugar sorter maintains a
 constant distance between the light source and the sensor regardless of the size of the fruit
 - → Decreased soluble solids content (SSC) measurement performance
- No studies have corrected this 'fruit size effect' in a physical way other than the preprocessing
 of the spectrum
- There is an attempt to develop SSC prediction model using deep learning (1D-Convolutional Neural Network) in addition to machine learning (Partial Least Squares, support vector machine), which has been widely used in the past.

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Research Purpose

- ➤ Determination of optimal light source and sensor distance by size in transmission spectroscopic analysis for predicting the SSC of apples
- > Development of 1D-CNN SSC prediction model using optimal distance



How the optical path changes depending on the size of the apple





2. Materials and Methods



2. Materials and Methods – Sample

- Apple : Fuji (Chungju agricultural products processing center (APC))
- Classification by weight : Level I ~VI, 411 apples

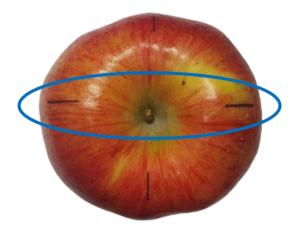
Size classification of apples in standard specifications of agricultural products in Korea

Level	I	п	ш	IV	V	VI
Weight(g)	375 ≥	300 ≥	250 ≥	214 ≥	188 ≥	167 ≥
weight(g)	373 <u>=</u>	375 <	300 <	250 <	214 <	188 <



		Level								
	I	I II III IV V								
Number	82	57	72	60	70	70				
Avg.(S.D.) Max. Diameter (mm)	99.16 (2.78)	90.17 (3.10)	88.23 (2.53)	80.8 (2.45)	78.92 (3.19)	75.63 (2.98)				
Avg.(S.D.) Weight (g)	398.02 (9.43)	318.41 (7.95)	285.16 (4.02)	223.19 (3.77)	194.55 (3.12)	182.28 (3.78)				





mark the maximum diameter of an apple



2. Materials and Methods – Equipment

Vis/NIR spectrometer

- USB4000, Ocean Optics, US
- Wavelength range: 472 1150 nm
- Resolution : about 0.2 nm

Light source

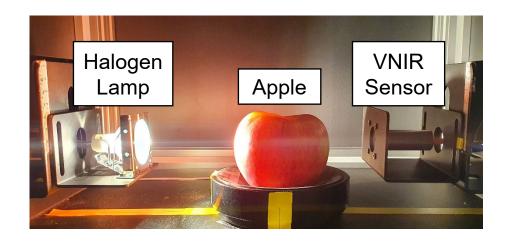
- 64637, OSRAM, Germany
- Tungsten-halogen light 100W 12V

Refractometer

PLA-3, ATAGO, Japan

• Brix scale : Brix 0.1%

• Accuracy : Brix ±0.1%



Spectroscopic measurement system



Measuring spectral data



2. Materials and Methods – Equipment

Vis/NIR spectrometer

- USB4000, Ocean Optics, US
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Refractometer

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- Brix scale : Brix 0.1%
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Optical fiber



Refractometer



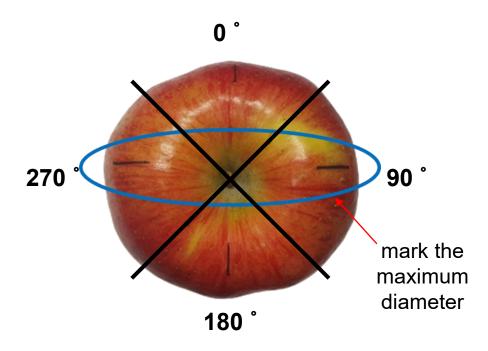
2. Materials and Methods – Equipment

Spectrum and SSC acquisition

Measurement area

: 0, 90, 180, 270 degree area of an apple

- Spectroscopic mode
 - Full-transmittance mode
- Spectroscopic condition
 - Integration Time: 100 msec
 - Spectra Averaged: 5 times



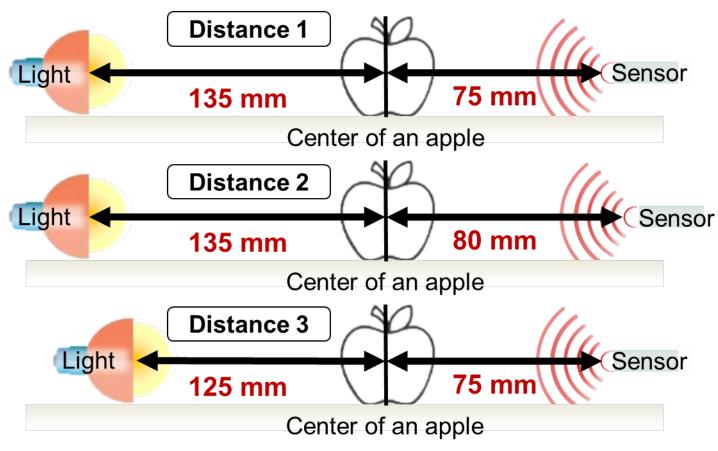
Measurement area of an apple





2. Materials and Methods – Design

Distance between light source - apple - sensor



3 optimal distances between light source – apple - sensor



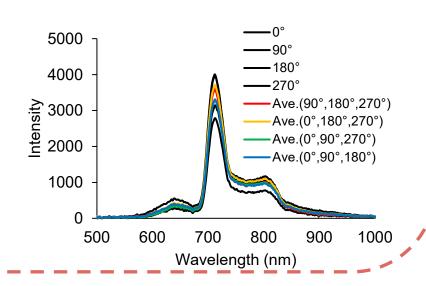


Spectral Preprocessing

- **Increasing** the number of spectra
 - Number of measured spectra by apple size: 228 ~ 328
 - Increase the number of spectra to avoid overfitting and improve performance on CNN

(Tian et al., 2022)

- : 4 spectra measured from 1 apple
- → Create new spectra by averaging 3 out of 4 spectra
- → A total of 8 spectra can be obtained from 1 apple





Spectral preprocessing

- Reduced
 - Reduce the resolution of the spectrum from 0.2 nm to 2 nm
 - → Noise cancellation, faster spectrum processing
- **Multiplicative scattering correction (MSC)**
 - Calibrating light scattering using an ideal spectrum (mean of spectra)
- Standard normal variable (SNV)
 - Calibrating light scattering using normalization of spectrum



2. Materials and Methods – 1D-CNN

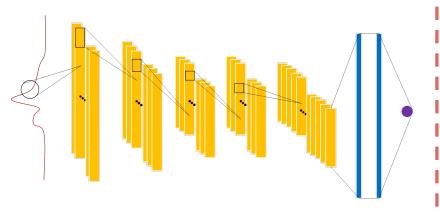
Development of SSC prediction model

- 1D-Convolutional Neural Network (1D-CNN)
 - One of the deep learning algorithms
 - Used a lot for image processing
 - Captures feature points of input data
 - 1D-CNN has 1D input data and filter on normal CNNs



Reference Architecture : AlexNet







1D-CNN architecture

Other setting values

Batch size: 14

Epoch: 300

EarlyStopping patience: 70

Input	Input shape : 456 ~ 656 x 1, Samples : 328,656
Conv 1D layer 1 + Relu	Filter size: 11 x 1, Stride: 4 Number of filters : 96, Padding: valid
Max pooling 1D 1	Pool size: 3 x 1, Stride: 2
BatchNormalization 1	
Conv 1D layer 2 + Relu	Filter size: 5 x 1, Stride: 1 Number of filters : 4, Padding: same
Max pooling 1D 2	Pool size: 3 x 1, Stride : 2
BatchNormalization 2	
Conv 1D layer 3 + Relu	Filter size: 3 x 1, Stride: 1
Conv 1D layer 4 + Relu	Number of filters : 384, Padding: same
Conv 1D layer 5 + Relu	Filter size: 3 x 1, Stride: 1 Number of filters : 256, Padding: same
Max pooling 1D 3	Pool size: 3 x 1, Stride : 2
Flatten	
Dense + Relu	Nodes: 4096
Dropout	Probability: 0.5
Dense + Relu	Nodes: 4096
Dropout	Probability: 0.5
Dense	Nodes: 1



Model Evaluation

• R_{pre}^2 (Coefficient of determination of prediction)

$$= \left(\frac{\sqrt{\sum_{i=1}^{n} (y_{pi} - y_{mean})^{2}}}{\sqrt{\sum_{i=1}^{n} (y_{mi} - y_{mean})^{2}}}\right)^{2}$$

• RMSEP (Root mean square error of prediction)

$$= \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_{pi} - y_{mi})^2}$$

 y_{pi} : Predicted SSC for the i-th apple

 y_{mi} : Measured SSC for the i-th apple

 y_{mean} : Average value of prediction set

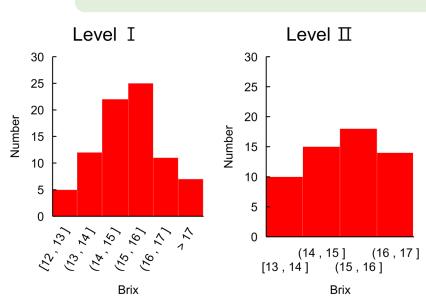
n: Number of prediction set

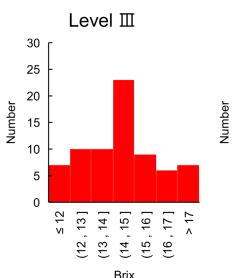


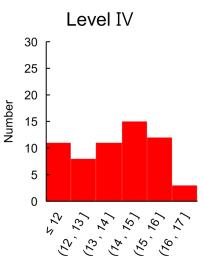


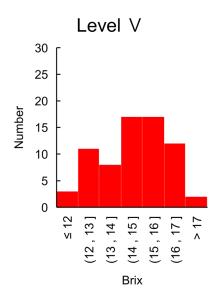


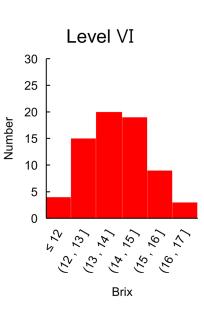
The distribution of the SSC of apples











Histogram of SSC distribution by Level

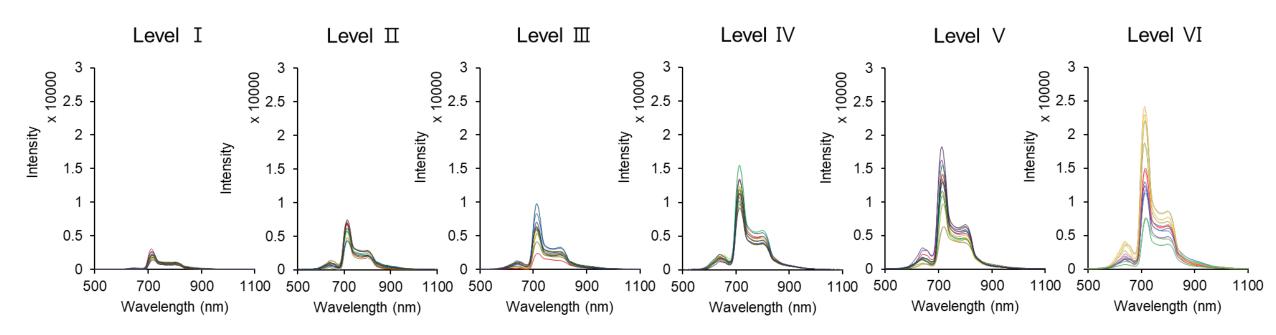
Table of SSC distribution by Level

			Level							
	I II III IV VI									
Num	Number		57	72	60	70	70			
SSC	Avg.	15.10	14.93	14.38	13.68	14.57	13.86			
(Brix)	SD	1.31	1.06	1.80	1.77	1.51	1.21			



[Distance 1] Transmission spectrum by apple size at light source 135 mm, sensor 75 mm





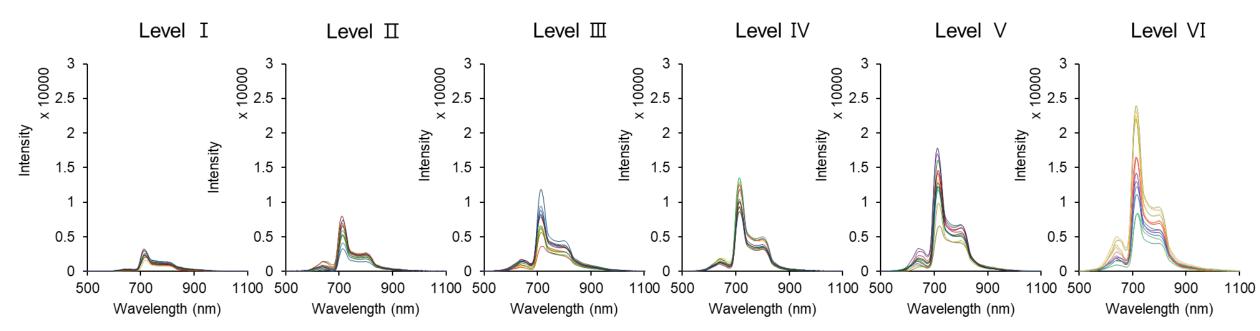
Measured transmission spectrum

- Larger apples tend to have smaller transmitted light intensity
- The distance of the light source has a greater influence on transmitted light intensity than the distance of the sensor



[Distance 2] Transmission spectrum by apple size at light source 135 mm, sensor 80 mm



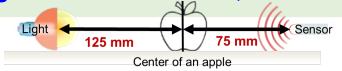


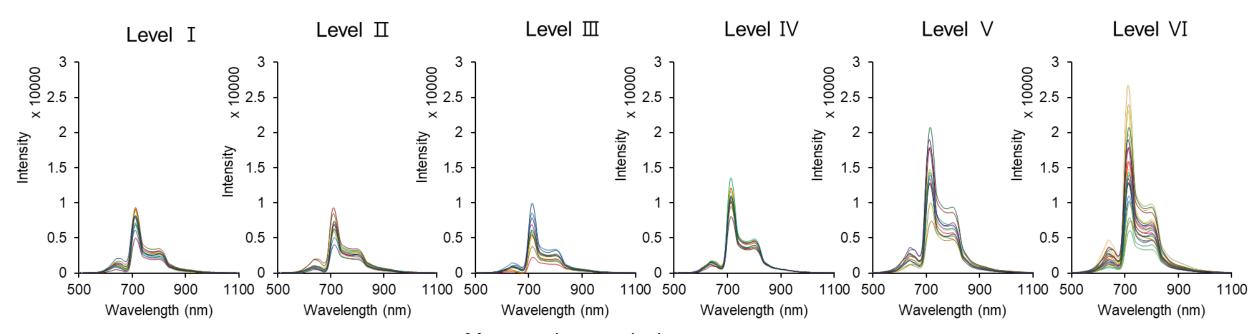
Measured transmission spectrum

- Larger apples tend to have smaller transmitted light intensity
- The distance of the light source has a greater influence on transmitted light intensity than the distance of the sensor



[Distance 3] Transmission spectrum by apple size at light source 125 mm, sensor 75 mm





- Measured transmission spectrum
- Larger apples tend to have smaller transmitted light intensity
- The distance of the light source has a greater influence on transmitted light intensity than the distance of the sensor



Performance of SSC prediction model by distance between light source and sensor

-Level I

Performance of the SSC prediction model of Level I

Level	Distance (Light - Sensor)	Preprocessing	Loss	Val_loss	RMSEC	R_{pre}^2	RMSEP
-		SNV	0.322	0.526	0.780	0.56	0.780
135	135 mm - 75 mm	MSC	0.287	0.391	0.579	0.76	0.579
- -	425 00	SNV	0.398	0.461	0.679	0.67	0.679
I 135 mm - 8	135 mm - 80 mm	MSC	0.333	0.325	0.500	0.82	0.500
	105 mans 75 mans	SNV	1.476	1.014	0.815	0.59	0.815
	120 Miii - 70 Mii	MSC	0.621	0.987	0.823	0.58	0.823

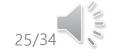


Optimal value

Preprocessing : MSC

 R_{pre}^2 : 0.82

• RMSEP: 0.500 Brix



Performance of SSC prediction model by distance between light source and sensor

- Level II

Performance of the SSC prediction model of Level II

Level	Distance (Light - Sensor)	Preprocessing	Loss	Val_loss	RMSEC	R_{pre}^2	RMSEP
•	135 mm - 75 mm	SNV	0.386	0.670	0.819	0.46	0.819
		MSC	0.364	0.279	0.519	0.78	0.520
	425	SNV	0.730	1.021	0.629	0.68	0.629
П	135 mm - 80 mm	MSC	0.322	0.643	0.725	0.58	0.725
125 mm - 75 mm	105 - 75 - 75	SNV	0.506	0.627	0.642	0.67	0.642
	MSC	1.745	1.314	0.904	0.35	0.904	



Optimal value

Preprocessing: MSC

 R_{pre}^2 : 0.78

• RMSEP: 0.520 Brix



Performance of SSC prediction model by distance between light source and sensor

- Level III

Performance of the SSC prediction model of Level III

Level	Distance (Light - Sensor)	Preprocessing	Loss	Val_loss	RMSEC	R_{pre}^2	RMSEP
_	405 75	SNV	0.416	0.697	0.770	0.83	0.769
1	135 mm - 75 mm	MSC	0.477	1.329	0.761	0.84 0.761	0.761
-	425 00	SNV	1.702	1.225	0.884	0.78	0.884
Ⅲ	135 mm - 80 mm	MSC	0.422	1.013	0.799	0.82	0.799
	125 mm - 75 mm	SNV	1.476	1.386	0.938	0.75	0.938
	125 mm - 75 mm	MSC	2.030	1.378	0.987	0.72	0.987

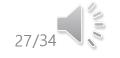


Optimal value

Preprocessing : MSC

 R_{pre}^2 : 0.84

• RMSEP: 0.761 Brix



Performance of SSC prediction model by distance between light source and sensor

- Level IV

Performance of the SSC prediction model of Level IV

Level	Distance (Light - Sensor)	Preprocessing	Loss	Val_loss	RMSEC	R_{pre}^2	RMSEP
-	425 75	SNV	0.461	0.607	0.779	0.84	0.779
	135 mm - 75 mm	MSC	0.403	0.930	0.765	0.85	0.765
T\ /	425 00	SNV	1.167	0.934	0.839	0.82	0.838
IV	135 mm - 80 mm	MSC	0.907	1.089	0.925		
	405 75	SNV	0.813	0.726	0.852	0.81	0.852
	125 mm - 75 mm	MSC	0.478	0.566 0.752	0.85	0.752	



Optimal value

Preprocessing: MSC

 R_{pre}^2 : 0.85

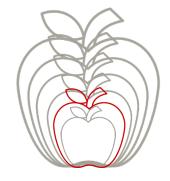
RMSEP: 0.752 Brix



- Performance of SSC prediction model by distance between light source and sensor
 - -Level V

Performance of the SSC prediction model of Level V

Level	Distance (Light - Sensor)	Preprocessing	Loss	Val_loss	RMSEC	R_{pre}^2	RMSEP
-	40E mana 7E mana	SNV	1.084	0.991	0.892	0.64	0.892
	135 mm - 75 mm	MSC	0.481	1.082	1.040	0.50	1.040
`	425 00	SNV	0.410	0.572	0.756	0.74	0.756
√ 135 mm - 80 ————————————————————————————————————	135 mm - 80 mm	MSC	0.516	1.349	0.810	0.70	0.810
	425 75	SNV	0.893	1.022	0.781	0.72	0.780
	125 mm - 75 mm	MSC	1.374	2.368	1.036	0.51	1.036



Optimal value

Preprocessing: MSC

 R_{pre}^2 : 0.74

• *RMSEP*: 0.756 Brix



Performance of SSC prediction model by distance between light source and sensor

- Level VI

Performance of the SSC prediction model of Level VI

Level	Distance (Light - Sensor)	Preprocessing	Loss	Val_loss	RMSEC	R_{pre}^2	RMSEP
-		SNV	0.670	0.563	0.624	0.75	0.624
135 mm - 75 mm	135 mm - 75 mm	MSC	1.121	0.763	0.797	0.58	0.797
\	425	SNV	0.837	0.656	0.693	0.69	0.693
VI	135 mm - 80 mm	MSC	1.872	1.740	0.902	0.47	0.902
	40E ways 7E ways	SNV	0.525	0.554	0.744	0.64	0.744
	125 mm - 75 mm	MSC	0.335	0.729	0.741	0.64	0.741

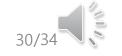


Optimal value

Preprocessing: MSC

 R_{pre}^2 : 0.75

• RMSEP: 0.624 Brix



Performance of SSC prediction model by distance between light source and sensor

- Total

Best performance of SSC prediction model by Level

Level	Distance (Light - Sensor)	Preprocessing	Loss	Val_loss	RMSEC	R_{pre}^2	RMSEP
I	135 mm - 80 mm	MSC	0.333	0.325	0.500	0.82	0.500
П	135 mm - 75 mm	MSC	0.364	0.279	0.519	0.78	0.520
Ш	135 mm - 75 mm	MSC	0.477	1.329	0.761	0.84	0.761
IV	125 mm - 75 mm	MSC	0.478	0.566	0.752	0.85	0.752
V	135 mm - 80 mm	SNV	0.410	0.572	0.756	0.74	0.756
VI	135 mm - 75 mm	SNV	0.670	0.563	0.624	0.75	0.624

Optimal Preprocessing

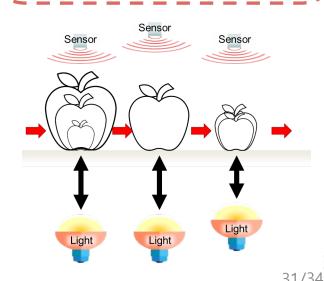
Large size : MSC

Small size: SNV

Optimal Value

 R_{pre}^2 : 0.74 ~ 0.85

RMSEP : 0.500 ~ 0.761 Brix





4. Conclusions

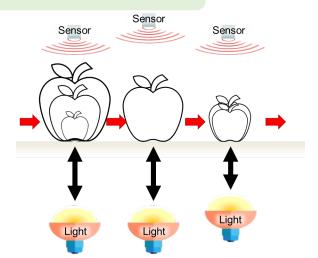


4. Conclusions

- Characterization of transmission spectrum by size of apple in transmission spectroscopy
 - ➤ Larger apples tend to have smaller transmitted light intensity
 - ➤ The distance of the light source has a greater influence on transmitted light intensity than the distance of the sensor

- Development of SSC prediction model of 3 distances of light source and sensor
 - ➤ The **distance** between the light source and the sensor representing optimal performance is **different for each level** of the apple
 - Optimal preprocessing varies by apple size

(large apple: MSC, small apple: SNV)



Thank you

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